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Author(s): Conlin, Jeremy Lloyd
Parsons, Donald K.
Gardiner, Steven J.
Gray, Mark G.
Lee, Mary Beth
White, Morgan C.
Kahler, Albert C. III

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Verification and Validation of the ENDF/B-VII.1-based Continuous Energy Data Tables for MCNP6

Jeremy Lloyd Conlin*, D. Kent Parsons, Steven J. Gardiner, Mark
Gray, A. C. Kahler, M. Beth Lee, and Morgan C. White

*Los Alamos National Laboratory
PO Box 1663, MS F663, Los Alamos, NM 87545*

Abstract — *In December 2011, the National Nuclear Data Center (NNDC) released ENDF/B-VII.1 [1], the “latest recommended evaluated nuclear data file for use in nuclear science and technology applications”. The data was released in the standard Evaluated Nuclear Data Format (ENDF) [2]. This release represents the advances made in nuclear data during the five years since the release of ENDF/B-VII.0 [3].*

The Nuclear Data Team at Los Alamos National Laboratory has processed the ENDF/B-VII.1 library and has made available a library of ACE data tables at several temperatures for each of the ENDF/B files. The ACE data library is called ENDF71x and is available through RSICC with MCNP6. The files can also be used with MCNP5 or other Monte Carlo codes.

*jlconlin@lanl.gov

I INTRODUCTION

In December 2011, the National Nuclear Data Center (NNDC) released ENDF/B-VII.1 [1], the “latest recommended evaluated nuclear data file for use in nuclear science and technology applications”. The data was released in the standard Evaluated Nuclear Data Format (ENDF) [2]. This release represents the advances made in nuclear data during the five years since the release of ENDF/B-VII.0 [3].

The Nuclear Data Team at Los Alamos National Laboratory has processed the ENDF/B-VII.1 library and has made available a library of ACE data tables at several temperatures for each of the ENDF/B files. The data was processed with the NJOY code [4], version 99.393. The lone exception is ^{35}Cl which was processed with NJOY version 2012. The ACE data library is called ENDF71x and has been distributed through RSICC along with MCNP6.

In 2008, the Nuclear Data Team at Los Alamos National Laboratory released an ACE library based upon ENDF/B-VII.0 [5]. The ENDF/B-VII.0 data files were processed with NJOY version 99.248 for five temperatures; 293.6 K, 600 K, 900 K, 1200 K and 2500 K. The data was made publicly available with the release of MCNP5 version 1.50. The ZAID suffixes associated with this data are 7xc with x ranging from 0–4, corresponding to the temperature of the ACE data table.

The release of the ENDF71x ACE data library includes all the ENDF/B-VII.1 evaluations processed at seven temperatures—the same five temperatures as in the ENDF/B-VII.0-based ACE library as well as 0.1 K and 250 K. The ENDF/B-VII.1 library contains evaluations for 423 nuclides. These, evaluated at seven temperatures each, provide 2961 ACE data tables.

I.A Changes in ENDF/B-VII.1 Since ENDF/B-VII.0

The ENDF/B-VII.1 paper by Chadwick et al. [1] states that the ENDF/B-VII.1 library contains advances in nine specific areas. For this paper the relevant advances are:

1. An increase in the breadth of neutron reaction cross section coverage, extending from 393 nuclides to 423 nuclides;
2. R-matrix analyses of neutron reactions on light nuclei, including isotopes of He, Li, and Be;
3. Resonance parameter analyses at lower energies and statistical high energy reactions for isotopes of Cl, K, Ti, V, Mn, Cr, Ni, Zr and W;
4. Modifications to thermal neutron reactions on fission products (isotopes of Mo, Tc, Rh, Ag, Cs, Nd, Sm, Eu) and neutron absorber materials (Cd, Gd);
5. Improved minor actinide evaluations for isotopes of U, Np, Pu, and Am (we are not making changes to the major actinides $^{235,238}\text{U}$ and ^{239}Pu at this point, except for delayed neutron data and covariances, and instead we intend to update them after a further period of research in experiment and theory), and our adoption of JENDL-4.0 evaluations for isotopes of Cm, Bk, Cf, Es, Fm, and some other minor actinides;
6. Fission energy release evaluations;
7. Fission product yield advances for fission-spectrum neutrons and 14 MeV neutrons incident on ^{239}Pu ; and

The ENDF/B-VII.1 library contains evaluations for 423 nuclides. The elemental evaluations for vanadium and zinc were replaced with isotopic evaluations and several other evaluations were added for a total of 32 new evaluations in ENDF/B-VII.1.

The evaluations that are new for ENDF/B-VII.1 are:

1. ^{50}V	12. ^{180}Ta	23. ^{240}Cm
2. ^{51}V	13. ^{180}W	24. ^{245}Bk
3. ^{64}Zn	14. ^{203}Tl	25. ^{246}Bk
4. ^{65}Zn	15. ^{205}Tl	26. ^{247}Bk
5. ^{66}Zn	16. ^{231}Th	27. ^{248}Bk
6. ^{67}Zn	17. ^{229}Pa	28. ^{246}Cf
7. ^{68}Zn	18. ^{230}Pa	29. ^{248}Cf
8. ^{70}Zn	19. ^{230}U	30. ^{251}Es
9. ^{168}Tm	20. ^{231}U	31. ^{252}Es
10. ^{169}Tm	21. ^{234}Np	32. $^{254m1}\text{Es}$;
11. ^{170}Tm	22. ^{240}Am	

or, given in ZA space:

1. 23050	12. 73180	23. 96240
2. 23051	13. 74180	24. 97245
3. 30064	14. 81203	25. 97246
4. 30065	15. 81205	26. 97247
5. 30066	16. 90231	27. 97248
6. 30067	17. 91229	28. 98246
7. 30068	18. 91230	29. 98248
8. 30070	19. 92230	30. 99251
9. 69168	20. 92231	31. 99252
10. 69169	21. 93234	32. 99654.
11. 69170	22. 95240	

I.B Modifications to ENDF/B-VII.1 in ENDF71x

While ENDF71x is based upon ENDF/B-VII.1 the Nuclear Data Team has made a few modifications to the original ENDF/B-VII.1 data. These changes were made as problems were found and corrected. Only the problems where the ENDF/B file could be easily changed were fixed; they are documented here. The other problems require more substantial changes to the ENDF/B file.

⁵⁶Fe In our visual inspection (see Section II.C) we found that the elastic scattering (MT=2) cross sections went to 0.0 b at an energy of 1.1971 MeV; when processed through NJOY, the resulting cross section value was 1×10^{-8} b. The elastic scattering and other important cross sections are shown in Figure 1a; it is clear that the very low cross section value is too small. We modified the ENDF/B file to replace the 0.0 b cross section with 1×10^{-6} b. This value for the cross section was chosen as the smallest reasonable value [6]. The modified ENDF/B file was processed to create an ACE data table. The new cross section plot is shown in Figure 1b.

⁶¹Ni Similarly to ⁵⁶Fe, ⁶¹Ni had some unreasonably small elastic scattering (MT=2) cross section values. The original ACE data table cross sections are shown in Figure 2a. The energies at which the elastic scattering cross section is unreasonably small are 0.742 925 1 MeV to 0.743 962 MeV and 0.818 412 0 MeV which corresponds to four cross section values that are too small. The ENDF/B file was modified—replacing the values that were too small with 1×10^{-6} —and reprocessed to create a new ACE data table. The modified cross sections are shown in Figure 2b. The cross sections are smaller than they were previously, but are still much smaller than the surrounding values. Additional work is required to properly correct the evaluation.

I.C ZA Identifiers

The nuclides in an ACE table are identified by their ZA plus an extension. The ZA plus the extension make up the ZA identifier or ZAID. The current ACE table format allows ten characters for a ZA and a suffix (ID); six digits indicating the ZA, a period, and a two-digit, one-character suffix. The ZAID looks like

$$\text{ZZZAAA.ddC}; \quad (1)$$

where

ZZZ the atomic number,

AAA the atomic mass number,

dd the library identifier,

T table type.

Note that ZZZ is blank padded, not zero padded if the atomic number is less than 100; e.g., ZZZ = 92 \neq 092 for uranium.

The formula for calculating the ZA for a particular nuclide is:

$$ZA = 1000 * Z + A, \quad (2)$$

where Z is the atomic number and A is the atomic mass number.

The formula for constructing the ZA, as given in Equation (2) has no way of indicating how to pick an evaluation based upon an excited state of an isotope. For excited state evaluations, we chose to follow the ZA construction used in the release of the ENDF/B-VII.0-based, ACE data tables [5]. For excited state evaluations, the formula for constructing a ZA is

$$ZA = 1000 * Z + 300 + s * 100 + A, \quad (3)$$

where s is the excited *state* of the evaluated isotopes; $s = 0$ for the ground state, $s = 1$ for the first excited state, etc. As an example, the ground and excited state ZAs for ^{58}Co are

27058	ground state
27458	first excited state

A historical exception to the ZA construction formulae given in Equations (2) and (3) is ^{242}Am . For many years, the first excited state for ^{242}Am was the only available evaluation and 95242 was used to identify it. The ground state evaluation was first made available in ENDF/B-VII.0. In order to maintain backwards compatibility, 95242 refers to the first excited state evaluation for ^{242}Am and 95642 refers to the ground state evaluation—the reverse of the convention.

I.D SZAX Identifiers

With the release of the ENDF/B-VII.1-based ACE data tables (2961 of them), the number of ACE data tables that ship with MCNP is nearly 10 600; more than half of them are incident neutron, continuous-energy data tables. Each data table must be uniquely identified. The number of available ZAID suffixes is diminishing. Because of the near exhaustion of ZAID suffixes, a change in the ZAID format is necessary to expand the number of unique identifiers available.

The Nuclear Data Team along with the MCNP and NJOY teams from LANL have developed an expanded identifier for ACE data tables which addresses the near exhaustion of ZAID extensions as well as providing an intuitive way to include excited state information in the identifier. The new identifier and the resulting modification to the ACE table header have been documented [7, 8].

The details will not be recounted here, but the definition of the new identifier is included.

The new formula for creating a unique identifier for a particular data table looks similar to the currently used ZAID;

$$\text{SSSZZZAAA.dddCC}, \quad (4)$$

where

SSS the excited state,
 ZZZ the atomic number,
 AAA the atomic mass number,
 ddd the library identifier,
 TT table type.

Like ZZZ, SSS is blank padded and not zero padded.

With the formula in Equation (4), the ground state evaluation keeps the traditional ZA and only the excited state evaluations have a new identifier. Note that since the excited state is now included, the name ZA is incomplete; we will refer to the new identifier as the SZA of the data table and SZAX when referring to the SZA and suffix as an extended version of the historic use of ZAID¹.

The new SZA can be constructed using the formula

$$\text{SZA} = \text{S} * 1\,000\,000 + \text{Z} * 1000 + \text{A}. \quad (5)$$

In addition to including the excited state as part of the SZAX, multiple characters can now be used in the suffix to indicate the class of data. For

¹As mentioned previously, ²⁴²Am will continue to be the anomaly with the SZA naming. The ground-state SZA will be 1095242 while the first excited-state will have an SZA of 95242.

example: incident neutron, continuous energy data, will use the characters `nc`. Continuing to use ^{58}Co as an example, the new SZAX would be

27058.710nc	ground state
1027058.710nc	excited state

ENDF71x ships with both the SZAX and ZAID style of identifying specific libraries. The ZA identifiers for the nuclides included in ENDF71x are given in Table 3. Table 2 shows the ZAs and SZAs for the excited state tables. (For ground state evaluations, the ZA and the SZAX are identical.)

The ZA suffixes for the ENDF71x are 8xc and the SZA extensions are 71xnc where `x` ranges from 0–6 and refers to the temperatures to which the evaluations were processed; 293.6 K, 600 K, 900 K, 1200 K, 2500 K, 0.1 K and 250 K respectively. Note, now there are three digits for the library identifier in the SZAX when there was just two in the ZAID. The ZA and SZA suffixes and their associated temperatures are shown in Table 1.

ZA Suffix	SZA eXtension	Temperature
80c	710nc	293.6 K
81c	711nc	600 K
82c	712nc	900 K
83c	713nc	1200 K
84c	714nc	2500 K
85c	715nc	0.1 K
86c	716nc	250 K

Table 1: Suffixes and temperatures for the nuclide identifier.

Warning. MCNP5 and MCNPX do not—and will not—understand a SZAX. In all of the beta releases and at least the first production version of MCNP6 will also not be able to properly handle a SZAX. Future versions of MCNP6

will be able to understand and properly use a SZAX instead of a ZAID.

For those versions of MCNP that can't use a SZAX, problems can arise if a SZAX is specified instead of a ZAID. If a user enters 92235.710nc (hoping for ENDF/B-VII.1-based, room temperature ^{235}U), MCNP5 will not crash, but will find and use 92235.71c (ENDF/B-VII.0-based, 600 K ^{235}U) instead. The SZAX entries will be the last ones in the `xsd` file and so are only found when the full SZAX is specified. Please make sure that what MCNP uses for its data is what you desired.

ZA	SZA
27458	1027058
47610	1047110
48515	1048115
52627	1052127
52529	1052129
61648	1061148
67566	1067166
95642	1095242 [*]
95242	95242 [†]
95644	1095244
99754	1099254

Table 2: ZA and SZA identifiers for the isotopes with excited-state data tables.

^{*}ground state of ^{242}Am

[†]first excited state of ^{242}Am

II VERIFICATION AND VALIDATION

We have performed an extensive amount of testing on the ENDF/B-VII.1-based ACE data tables, more than any previous ACE data release from the Nuclear Data Team at LANL. We have verified our data through a series of small scripts and programs and we have performed simple verification by using our data in “mechanical” calculations in MCNP.

1001	1002	1003	2003	2004	3006	3007	4007*	4009	5010
5011	6000	7014	7015	8016	8017	9019	11022	11023	12024
12025	12026	13027	14028	14029	14030	15031	16032	16033	16034
16036	17035	17037	18036	18038	18040	19039	19040	19041	20040
20042	20043	20044	20046	20048	21045	22046	22047	22048	22049
22050	23050*	23051*	24050	24052	24053	24054	25055		
26054	26056	26057	26058	27058	27059	27458	28058	28059	28060
28061	28062	28064	29063	29065	30064*	30065*	30066*	30067*	30068*
30070*	31069	31071	32070	32072	32073	32074	32076	33074	33075
34074	34076	34077	34078	34079	34080	34082	35079	35081	36078
36080	36082	36083	36084	36085	36086	37085	37086	37087	38084
38086	38087	38088	38089	38090	39089	39090	39091	40090	40091
40092	40093	40094	40095	40096	41093	41094	41095	42092	42094
42095	42096	42097	42098	42099	42100	43099	44096	44098	44099
44100	44101	44102	44103	44104	44105	44106	45103	45105	46102
46104	46105	46106	46107	46108	46110	47107	47109	47111	47510
48106	48108	48110	48111	48112	48113	48114	48116	48515	49113
49115	50112	50113	50114	50115	50116	50117	50118	50119	50120
50122	50123	50124	50125	50126	51121	51123	51124	51125	51126
52120	52122	52123	52124	52125	52126	52128	52130	52132	52529
52527	53127	53129	53130	53131	53135	54123	54124	54126	54128
54129	54130	54131	54132	54133	54134	54135	54136	55133	55134
55135	55136	55137	56130	56132	56133	56134	56135	56136	56137
56138	56140	57138	57139	57140	58136	58138	58139	58140	58141
58142	58143	58144	59141	59142	59143	60142	60143	60144	60145
60146	60147	60148	60150	61147	61148	61149	61151	61548	62144
62147	62148	62149	62150	62151	62152	62153	62154	63151	63152
63153	63154	63155	63156	63157	64152	64153	64154	64155	64156
64157	64158	64160	65159	65160	66156	66158	66160	66161	66162
66163	66164	67165	67566	68162	68164	68166	68167	68168	68170
69168*	69169*	69170*	71175	71176	72174	72176	72177	72178	72179
72180	73180*	73181	73182	74180*	74182	74183	74184	74186	75185
75187	77191	77193	79197	80196	80198	80199	80200	80201	80202
80204	81203*	81205*	82204	82206	82207	82208	83209	88223	88224
88225	88226								
89225	89226	89227	90227	90228	90229	90230	90231*	90232	90233
90234	91229*	91230*	91231	91232	91233	92230*	92231*	92232	92233
92234	92235	92236	92237	92238	92239	92240	92241	93234*	93235
93236	93237	93238	93239	94236	94237	94238	94239	94240	94241
94242	94243	94244	94246	95240*	95241	95242	95243	95244	95642
95644	96240*	96241	96242	96243	96244	96245	96246	96247	96248
96249	96250	97245*	97246*	97247*	97248*	97249	97250	98246*	98248*
98249	98250	98251	98252	98253*	98254	99251*	99252*	99253*	99254
99255	99654*	100255							

Table 3: List of ZAs for the ACE data tables released with ENDF71x. The separations are merely for convenience and show the light ($Z < 25$), mid-weight ($25 \leq Z < 89$) and the actinides. The ZAs with an asterisk (*) indicate isotopes new to ENDF/B-VII.1 and ZAs new in the ENDF71x library.

We have also performed a visual inspection of the room temperature cross sections for these five reactions:

1. total,
2. absorption,
3. elastic scattering,
4. $(n, 2n)$,
5. fission, and
6. average heating number.

The purpose of the visual inspection was to find gross errors in the cross section values. Neither running the data through MCNP nor checking the data with our scripts are capable of finding these kinds of errors—this requires some knowledgeable human inspection.

These three verification and validation tasks ensure that the ENDF71x library is the most heavily verified and validated library ever released by the Nuclear Data Team at Los Alamos National Laboratory. In this section, we present our findings from the three verification and validation tasks that we have performed.

Verification and validation is extremely important to the Nuclear Data Team. We recognize the trust that is placed on our data and know that once the data has been distributed there is no mechanism to recall the data if a problem is found. The verification process is described in Section II.A with the validation process described in Section II.B.

With that being said, we are somewhat at the mercy of the data evaluators, those who create the ENDF/B data files. If the ENDF/B data is wrong, or malformed, we are limited in the corrections we can provide. We can, however, raise a warning when issues arise. In general, the ENDF/B-VII.1 data release is of the highest quality that can be found and thus, there are few cases where

the data is suspect.

*II.A Verification of Data with **checkace***

The Nuclear Data Team at LANL have developed a series of small programs used to verify the quality of ACE data tables. These small programs are driven by a script called **checkace**. This script and programs were run on all of the room temperature ACE data tables with the assumption being made that checking just the room temperature cases would find the problems in the remaining temperatures—there wouldn't be anything found in the higher temperature data tables that wouldn't be caught in the room temperature data. The only change in the processing between temperatures was the input of the desired temperature so additional problems should not be introduced simply by changing the temperature on the NJOY input card(s).

The kinds of errors that **checkace** looks for are:

- non-leading zero in threshold reactions;
- properly formatted MT=5 threshold reactions;
- negative PDFs for secondary neutron energy distributions;
- negative or zero-value heating numbers;
- negative secondary discrete photon energies for MT=4 or MT=44;
- unphysical secondary neutron energies;
- unphysical Q-values in threshold reactions;
- sum of partial cross-sections does not equal total cross section.

The majority of these checks did not turn up anything significant. Some of them exposed errors that turned out to be related to computer round-off errors, but not anything of significance. The noteworthy errors are detailed next

Negative PDF Values In the ^{153}Eu evaluation, unphysical, negative PDF values were found for secondary neutrons for the MT=91 reaction. These negative values originate in the ENDF/B-VII.1 evaluation and are not a consequence of NJOY processing. We truncated the negative PDF values and made all of them 0.0. As a result, the total PDF sums to greater than 1.0.

The MT=91 reaction is (n, n') and is not common. We don't anticipate the truncation of negative PDF values for this reaction to have a major impact on calculations.

Heating Calculation Problems There were problems with the heating values in 41 of our data tables. The problem evaluations are:

1. ^{33}S	15. $^{115m1}\text{Cd}$	29. ^{168}Tm
2. ^{36}S	16. ^{132}Te	30. ^{174}Hf
3. ^{59}Ni	17. ^{529}Te	31. ^{176}Hf
4. ^{92}Zr	18. ^{143}Ce	32. ^{177}Hf
5. ^{93}Zr	19. ^{145}Nd	33. ^{178}Hf
6. ^{94}Zr	20. ^{147}Nd	34. ^{179}Hf
7. ^{95}Zr	21. ^{147}Sm	35. ^{180}Hf
8. ^{96}Zr	22. ^{149}Sm	36. ^{197}Au
9. ^{93}Nb	23. ^{151}Sm	37. ^{196}Hg
10. ^{92}Mo	24. ^{153}Gd	38. ^{202}Hg
11. ^{94}Mo	25. ^{155}Gd	39. ^{203}Tl
12. ^{96}Mo	26. ^{165}Ho	40. ^{205}Tl
13. ^{97}Mo	27. ^{566}Ho	41. ^{209}Bi
14. ^{98}Mo	28. ^{166}Er	

Negative heating values may cause problems with energy deposition or kerma calculations. We don't anticipate the problems with the negative heating values

in ENDF71x to drastically alter calculations, but the user should be aware of the problems.

When negative (or zero) values of the heating value are plotted on log-log plot (as is typically done for cross sections), a gap is seen in the plot. An example of a gap in the average heating values can be seen in Figure 3 where a large gap in the average heating value can be seen around 1 MeV.

Independently, MacFarlane [9, 10], found a number of problems with kerma values, average heating, and missing photon energy production. Every calculation that we found to be problematic was also found to be problematic by MacFarlane as well. These are problems with the original ENDF/B-VII.1 file and corrections need to be made there. Please see MacFarlane’s work at <http://t2.lanl.gov/data/endl/ebalVII/summary.html>.

Sum of Partial Unresolved Resonance Cross-Sections Don’t Equal Total

There were 15 evaluations that had significant problems with their unresolved resonance probability tables. These evaluations were reprocessed by NJOY without using the PURR module; the cross section values for the unresolved resonance range in the ACE data table are the average cross section values given in MF=3 of the ENDF/B file. The evaluations that we processed without using the PURR module are:

- | | | |
|---------------------|-----------------------|-----------------------|
| 1. ^{22}Na | 6. ^{106}Cd | 11. ^{232}U |
| 2. ^{36}Ar | 7. ^{170}Tm | 12. ^{236}Pu |
| 3. ^{58}Co | 8. ^{182}W | 13. ^{249}Bk |
| 4. ^{65}Zn | 9. ^{186}W | 14. ^{249}Cf |
| 5. ^{70}Ge | 10. ^{203}Tl | 15. ^{250}Cf |

II.B Validation through Mechanical Testing With MCNP6 and MCNP5

A number of “mechanical” tests have been performed to ensure—at the very least—that the ACE data tables don’t cause MCNP to crash. These tests consisted of four fixed-source calculations that were performed for every combination of nuclide and temperature available in ENDF71x using both MCNP6 and MCNP5. The density for these problems was the nominal density of the element or 1 g cm^{-3} if the nominal density was less than 1 g cm^{-3} .

Three fixed-source calculations were performed using an isotropic point neutron source at the origin surrounded by a uniform sphere (4 cm radius) composed of a single nuclide. The three energy spectrums simulated are:

- 1) a log-uniform distribution on the entire interval spanned by the energy grid of the appropriate ACE file,
- 2) a Watt fission spectrum, or
- 3) a room-temperature Maxwell-Boltzmann distribution.

A fourth fixed-source calculation used the same log-uniform distribution of neutron energies as the first, but the source was uniformly distributed throughout the volume of the sphere. Neutrons and secondary photons (i.e., `mode n p`) were transported in these calculations.

Tallies of the current across the outer surface of the sphere (MCNP F1 tally), the flux at the outer surface of the sphere (MCNP F2 tally), and the average flux within the sphere (MCNP F4 tally) were performed for both neutrons and photons. Each tally was binned into 500 logarithmically-spaced energy bins. The neutron tallies covered the entire energy range for which cross section data exists for a given isotope in ENDF71x, while for photon tallies the lower end of this energy range was truncated at 1 keV, the minimum cutoff energy for photons

in MCNP. One billion source neutrons were tracked in each calculation, and no computer time limit was imposed.

II.B.1 Data Issues Affecting MCNP Execution

During our mechanical testing of the ENDF71x data tables, we discovered two issues with the ACE data tables that caused MCNP to crash. Our investigation of these problems revealed that they are symptomatic of issues that affect MCNP5, MCNPX and earlier versions of MCNP.

Law 4 Data describing secondary energy distributions in ENDF/B are formatted according to “laws”. These are not physical laws, merely formats that describe the physics. We have found an inconsistency with the ENDF/B data formatted with law 4. Law 4 represents the distribution of secondary photon energies for a reaction using a table of incident neutron energies. For each incident neutron energy given on the table, the secondary photon energy distribution may be represented using discrete lines, a continuum, or both. MCNP requires that the same number of secondary discrete energies on an ACE data table for every incident energy. A continuous distribution of secondary energies may also be defined.

ENDF/B-VII.1 introduced some reactions that had a discrete representation, but no continuous distribution. MCNP assumes that there will always be a distribution in addition to the discrete photon lines. MCNP6 has been updated to handle situations where there may not be a continuous distribution of photon energies. Although very rare, use of ENDF/B-VII.1-based ACE data tables in MCNP5, MCNPX or earlier versions of MCNP may result in MCNP crashing if this specific data representation is encountered. More information about this problem can be found in the technical report by Kiedrowski et al. [11].

This problem occurs for photons emitted from (n, xn) reactions in the fol-

lowing minor actinides:

1. ^{226}Ac	11. ^{246}Pu	21. ^{250}Cf
2. ^{227}Th	12. ^{243}Cm	22. ^{251}Cf
3. ^{228}Th	13. ^{245}Cm	23. ^{252}Cf
4. ^{230}Th	14. ^{247}Cm	24. ^{253}Cf
5. ^{233}Th	15. ^{248}Cm	25. ^{254}Cf
6. ^{234}Th	16. ^{249}Cm	26. ^{252}Es
7. ^{230}Pa	17. ^{246}Bk	27. ^{253}Es
8. ^{232}U	18. ^{248}Bk	28. ^{255}Es
9. ^{235}Np	19. ^{249}Bk	
10. ^{242}Pu	20. ^{246}Cf	

For all of these nuclides, the problematic law 4 data were added in the ENDF/B-VII.1 release which were borrowed from JENDL-4.0 [12].

Unphysical Number of Secondary Neutrons for in Protactinium The MT=5 reactions in ^{231}Pa and ^{233}Pa have a problem with the secondary neutron yield. MT=5 is a catch-all reaction that represents everything not already accounted for in the other reactions. For the MT=5 reactions in ^{231}Pa and ^{233}Pa , the secondary neutron yields for incident energies greater than 20 MeV are unrealistically large—see Figure 4. These unphysical neutron yields were added in ENDF/B-VII.0 and remain unchanged in ENDF/B-VII.1.

All currently extant versions of MCNP assume that the number of secondary neutrons produced by a single instance of certain reactions will never exceed 11—a reasonable assumption. When more than 11 secondaries are produced MCNP modifies data beyond the array bounds which eventually results in a segmentation fault. The number of secondary neutrons produced in the MT=5 reaction in $^{231,233}\text{Pa}$ is clearly incorrect. Fortunately $^{231,233}\text{Pa}$ is not a major

isotope and MT=5 is also a rare event—this problem won’t occur very often. Future releases of ENDF/B should fix the data.

II.C Visual Inspection of Major Cross Sections

The previous sections have shown how we have attempted to find problems with the data using checking codes and running simulations. However, there are some things that can only be found by the human eye.

We have plotted these reactions: 1) total, 2) absorption, 3) elastic scattering, 4) $(n, 2n)$, 5) fission, and 6) average heating number (kerma times total cross section). These data were chosen to be plotted because they are important reactions or because we have had complications with them in the past. The data was taken from our ACE data tables, but originates in the ENDF/B-VII.1 evaluation files.

The cross sections were plotted *for every evaluation* and we have visually inspected every plot looking for errors in the data. This inspection was intended to catch gross errors and not the small problems that might occur. We explain our findings from the visual inspection in the following paragraphs.

Sawtooth Cross Sections We found a number of evaluations with changes in the cross section value of several orders of magnitude. These large unphysical changes appear to have a “sawtooth” in the plot of the cross section. The large change in the cross section is not limited to the ACE data tables, but is an issue with the ENDF/B-VII.1 files themselves.

A typical example of the sawtooth-like pattern is shown in Figure 5 where we can see a large drop in the cross sections at a little less than an eV. A list of evaluations that have this pattern is given here.

1. ^{58m1}Co	22. ^{131}I	43. ^{229}Pa
2. ^{65}Zn	23. ^{124}Xe	44. ^{230}U
3. ^{79}Se	24. ^{133}Xe	45. ^{231}U
4. ^{78}Kr	25. ^{134}Xe	46. ^{241}U
5. ^{89}Sr	26. ^{136}Cs	47. ^{235}Np
6. ^{90}Sr	27. ^{137}Cs	48. ^{239}Np
7. ^{91}Y	28. ^{144}Ce	49. ^{246}Pu
8. ^{95}Nb	29. ^{148}Pm	50. ^{243}Am
9. ^{99}Mo	30. ^{149}Pm	51. ^{240}Cm
10. ^{96}Ru	31. ^{156}Eu	52. ^{241}Cm
11. ^{98}Ru	32. ^{223}Ra	53. ^{249}Cm
12. ^{105}Ru	33. ^{224}Ra	54. ^{245}Bk
13. ^{106}Ru	34. ^{225}Ra	55. ^{247}Bk
14. ^{105}Rh	35. ^{225}Ac	56. ^{248}Cf
15. ^{123}Sn	36. ^{226}Ac	57. ^{251}Cf
16. ^{126}Sn	37. ^{227}Ac	58. ^{253}Cf
17. ^{124}Sb	38. ^{227}Th	59. ^{254}Cf
18. ^{125}Sb	39. ^{228}Th	60. ^{251}Es
19. ^{120}Te	40. ^{231}Th	61. ^{254}Es
20. $^{129m1}\text{Te}$	41. ^{233}Th	62. ^{255}Es
21. $^{127m1}\text{Te}$	42. ^{234}Th	

Average Heating Gaps Another problem discovered in the visual inspection of the cross sections is gaps in the average heating value. Because the data is plotted on a log scale, a gap is seen if the average heating value is less than or equal to zero.

A typical example of the gap in the average heating values was shown previ-

ously in Figure 3 where a large gap in the average heating value is seen around 1 MeV. The list of evaluations that have this pattern is given below. The heating problems shown in these evaluations have been confirmed by Bob MacFarlane [10, 9]

1. ^{33}S	14. ^{97}Mo	27. ^{177}Hf
2. ^{36}S	15. ^{98}Mo	28. ^{178}Hf
3. ^{39}K	16. $^{115m1}\text{Cd}$	29. ^{179}Hf
4. ^{59}Ni	17. ^{132}Te	30. ^{180}Hf
5. ^{92}Zr	18. ^{143}Ce	31. ^{197}Au
6. ^{93}Zr	19. ^{147}Sm	32. ^{196}Hg
7. ^{94}Zr	20. ^{149}Sm	33. ^{199}Hg
8. ^{95}Zr	21. ^{151}Sm	34. ^{202}Hg
9. ^{96}Zr	22. $^{166m1}\text{Ho}$	35. ^{203}Tl
10. ^{93}Nb	23. ^{166}Er	36. ^{205}Tl
11. ^{92}Mo	24. ^{168}Tm	37. ^{209}Bi
12. ^{94}Mo	25. ^{174}Hf	
13. ^{96}Mo	26. ^{176}Hf	

Unphysically Small Elastic Scattering Cross Sections Two evaluations— ^{56}Fe and ^{61}Ni —had elastic scattering (MT=2) cross sections that were much too small. Upon closer inspection of the ENDF/B file, we discovered that the cross sections went to 0.0 which we don’t believe is accurate. The ENDF/B files for these two isotopes were modified as explained in Section I.B.

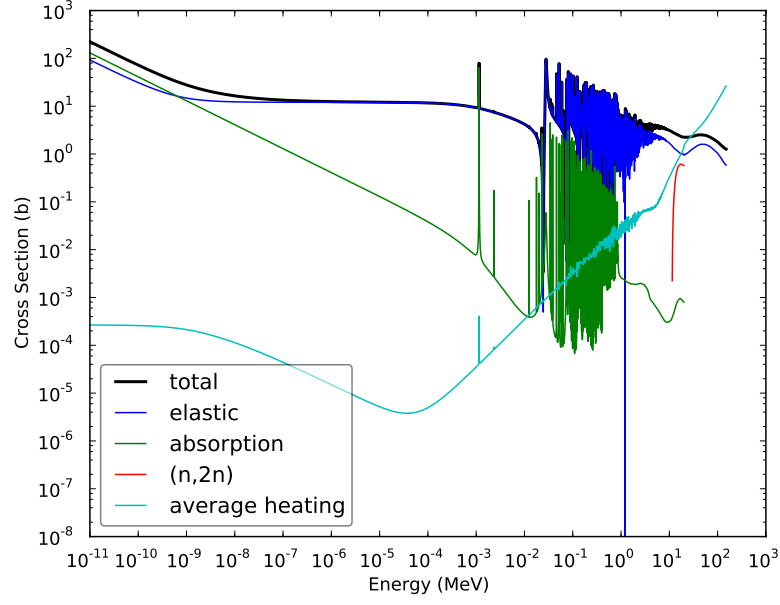
Unphysically Large Elastic Scattering Cross Sections In contrast to the small elastic scattering cross sections in ^{56}Fe and ^{61}Ni , we feel that the elastic scattering (MT=2) cross sections in ^{237}U and ^{238}Pu are unphysically large. This is a deficiency in the ENDF/B-VII.1 evaluation file and not a result of our

processing.

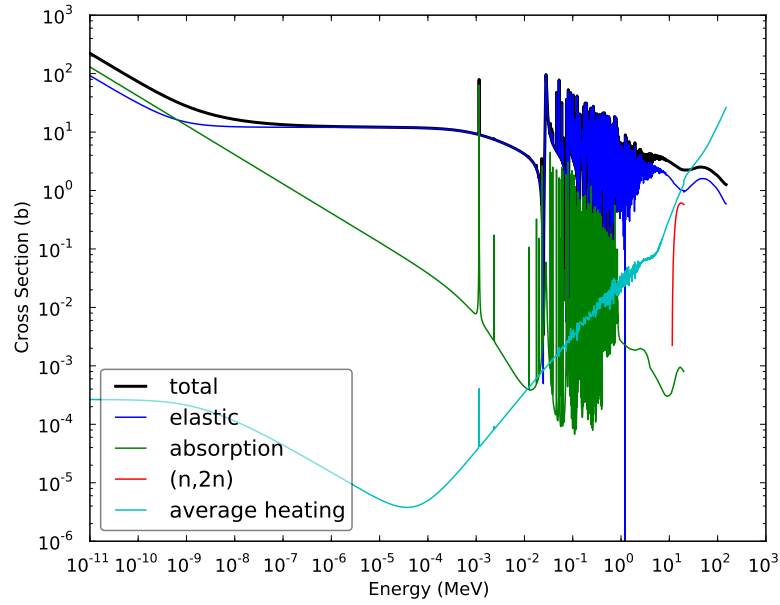
III CONCLUSION

The Nuclear Data Team at Los Alamos National Laboratory has made available a library—called ENDF71x—of continuous-energy, ACE data tables suitable for use with Monte Carlo codes. The data is based on ENDF/B-VII.1, with two small modifications to ^{56}Fe and ^{61}Ni . The ENDF/B-VII.1 evaluation files were processed using NJOY version 99.393

The ENDF71x library has been verified and validated to ensure the data is physically correct, and properly formatted so that computer codes can accurately use the data.

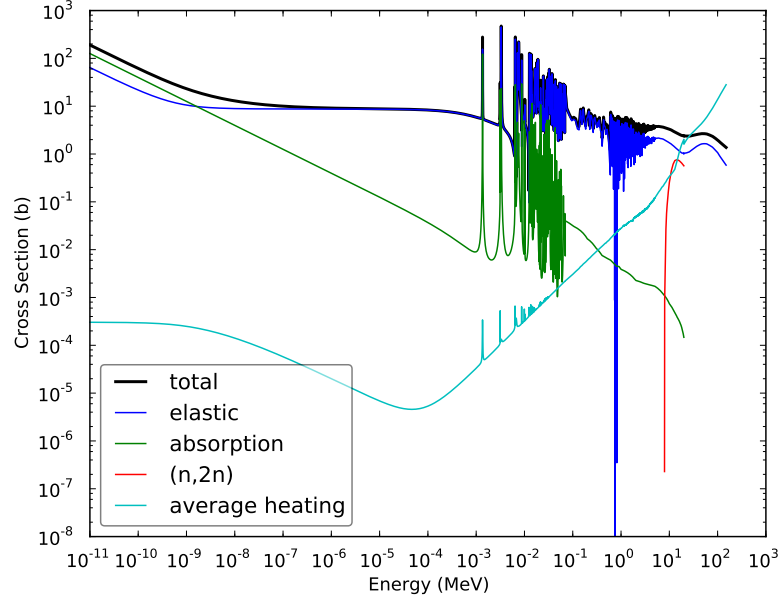


(a) Unmodified ENDF/B-VII.1 data.

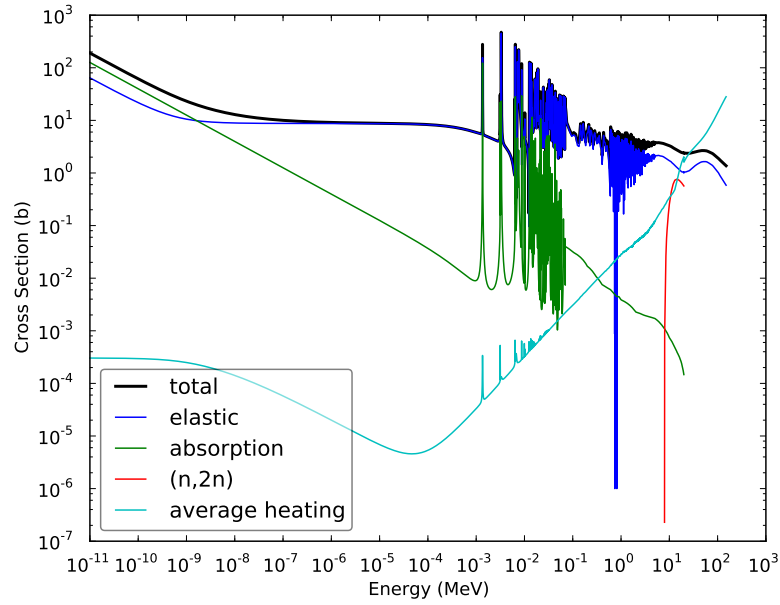


(b) Modified ENDF/B-VII.1 data.

Figure 1: Cross section plot of the total, elastic, absorption, and $(n, 2n)$ cross sections of ^{56}Fe as well as the average heating. Note the difference in scales of the ordinates.



(a) Unmodified ENDF/B-VII.1 data.



(b) Modified ENDF/B-VII.1 data.

Figure 2: Cross section plot of the total, elastic, absorption, and $(n, 2n)$ cross sections of ^{61}Ni as well as the average heating.

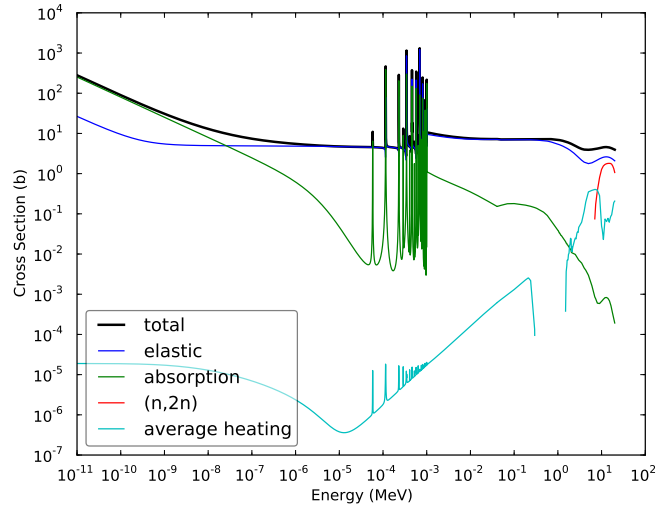


Figure 3: Plot of the “major” $^{115m1}\text{Cd}$ cross sections showing the unphysical gaps in the average heating value around 1 MeV.

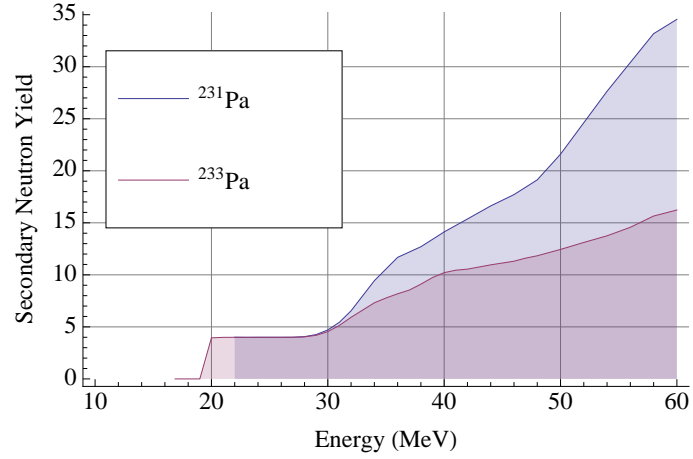


Figure 4: Plot of the ^{231}Pa (blue) and ^{233}Pa (purple) secondary neutron yields for MT=5 showing the unphysical values above about 30 MeV.

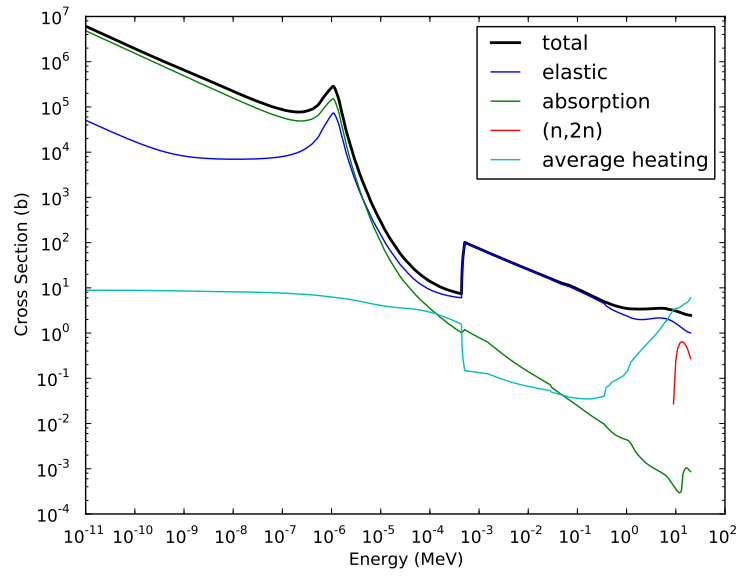


Figure 5: Plot of the “major” ^{58m1}Co cross sections showing the unphysical, sawtooth-like problem.

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